



Formula: C<sub>30</sub>H<sub>28</sub>O<sub>12</sub>

MW: 580.55

CAS: 84813-73-0

MDL:

TNP:



LogP: -1.06

LogS: -3.11

Acceptors: 12

Donors: 6

Rotation Bonds: 12

Chiral Centers: 6

N+O: 12

LIPINSKY: 1

IUPAC: 2-[(2S)-5-hydroxy-2-(4-hydroxyphenyl)-4-oxochroman-7-yloxy]-4,5-dihydroxy-6-(hydroxymethyl)-2H-3,4,5,6-tetrahydropyran-3-yl (2E)-3-(4-hydroxyphenyl)prop-2-enoate

Smiles:

c1(ccc(cc1)O)/C=CC(OC1C(C(C(OC1Oc1cc2c(C(C[C@H](O2)c2ccc(cc2)O)=O)c(O)c1)CO)O)O)=O

REFERENCE: M. P. Yuldashev,